

ESTIMATION OF BOND PERCOLATION THRESHOLDS ON THE ARCHIMEDEAN LATTICES

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ABSTRACT. We give accurate estimates for the bond percolation critical probabilities on seven Archimedean lattices, for which the critical probabilities are unknown, using an algorithm of Newman and Ziff.

1. INTRODUCTION

Since the introduction of percolation theory, it has been an interesting and challenging problem to determine the percolation thresholds. Only a few non-trivial graphs are exactly solved, such as the bond model on the square, triangular and hexagonal lattices, and the site model on the triangular and Kagomé lattices. Recently Scullard and Ziff have found many new thresholds for various classes of lattices [6, 9]. They also conjecture, [10], the value of the threshold for one lattice considered here: the $(3, 12^2)$ lattice, and also for the Kagomé lattice. Precise estimates have been calculated for example for the site model on the Archimedean lattices, [7], and for the bond model on the Kagomé lattice, [11].

Bounds, more or less tight, have been found by various authors for some lattices. For the bond model on the Archimedean lattices, see [4] for a review of rigorous bounds on critical probabilities. Recently, Riordan and Walters, [5], have given tight rigorous confidence intervals for both site and bond percolation on all Archimedean lattices.

In this paper, we provide precise estimates for the bond percolation thresholds for the unsolved Archimedean lattices.

1.1. Archimedean lattices. The Archimedean lattices are the vertex transitive graphs that can be embedded in the plane such that every face is a regular polygon. A polygon is regular if all edges have the same length, and all interior angles are the same. Kepler, [1], showed that there exists exactly 11 such graphs.

The lattices are given names according to the sizes (number of sides of the polygon) of faces incident to a given vertex. The face sizes are listed in order, starting with a face such that the list is the smallest possible in lexicographical order. The square lattice thus gets the name $(4, 4, 4, 4)$, abbreviated to (4^4) , and the Kagomé lattice the name $(3, 6, 3, 6)$.

Square representations of the Archimedean lattices studied here, are shown in Figure 1.

The bond percolation threshold is known exactly for the square, triangular, and hexagonal lattices (the values are 0.5 , $2 \sin(\frac{\pi}{18})$, and $1 - 2 \sin(\frac{\pi}{18})$), and the threshold for the Kagomé lattice has previously been estimated to $0.524\,4053$ by Ziff and Suding, [11]. Ziff

and Scullard's, [10] conjectured value for $(3, 12^2)$ is $0.740\,421\,178\dots$, and it is consistent with the estimate given here: $0.740\,4219$ (8) — the difference is less than one standard deviation (further, there is a small positive bias in the estimate).

In this work we estimate the thresholds for all the Archimedean lattices with unknown (and in one case conjectured) threshold except the previously studied Kagomé lattice. The hexagonal lattice is used as a benchmark.

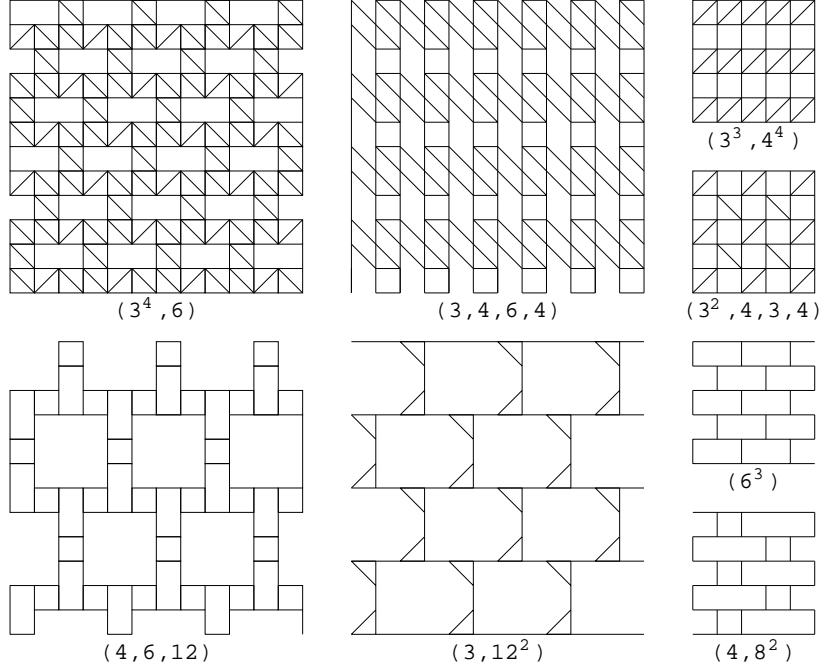


FIGURE 1. Finite subgraphs of square embeddings of 8 Archimedean lattices.

1.2. Percolation. The bond percolation process is defined as follows. For each edge of a graph G , declare the edge to be open with probability p , independently of all other edges, and closed otherwise.

For the kind of graphs studied here, it is well known that there exists a critical value $p_c(G)$, called the critical probability, or threshold, such that for $p > p_c(G)$, there exists a unique infinite connected component of open edges, while for $p < p_c(G)$, only finitely large connected components of open edges exist.

1.3. Motivation. One objective of this simulation study is to get an empirical answer to the following question.

Question 1.1. *If G and H are two Archimedean lattices, with self-avoiding walk connective constants $\mu(G)$ and $\mu(H)$, site percolation thresholds $p_c^s(G)$ and $p_c^s(H)$, and bond percolation thresholds $p_c^b(G)$ and $p_c^b(H)$, is it true that*

$$\mu(G) \leq \mu(H) \Leftrightarrow p_c^s(G) \geq p_c^s(H) \Leftrightarrow p_c^b(G) \geq p_c^b(H).$$

The answer is negative for general two dimensional, quasi-transitive, planar graphs, as shown by Wierman, [8], and Parviainen, [3].

Available estimates and rigorous bounds for site percolation thresholds and connective constants suggest that these two models give the same order on the Archimedean lattices.

The estimates given in this work suggest, however, that there exist two pairs of Archimedean lattices for which the bond and site percolation thresholds are in opposite order, namely the pair $(3, 6, 3, 6)$ (Kagomé) and $(3, 4, 6, 4)$ (Ruby), and the pair $(3^3, 4^2)$ and $(3^2, 4, 3, 4)$.

2. THE METHOD OF NEWMAN AND ZIFF

Newman and Ziff, [2], have developed a fast algorithm for estimating percolation thresholds (both bond and site); the running time is nearly *linear* in the system size (the number of vertices or edges of the subgraph), while still producing accurate estimates.

It turns out that it is profitable to modify the subgraphs used, and use torus shaped regions. We will consider $Q(p)$, the probability that a cluster wraps around the torus in one direction, but not both.

If we generate a percolation process on a subgraph with M edges, by adding edges in random order, we get $M + 1$ different, but dependent, realizations of a percolation process. These give a rough estimate of the function $q(n)$, the probability that a cluster spans the torus in one direction but not the other, given that there are exactly n open edges.

Assume for the moment that $q(n)$ is exactly known. The law of total probability then gives us $Q(p)$:

$$Q(p) = \sum_{n=0}^M q(n) \binom{M}{n} p^n (1-p)^{M-n}.$$

Thus from a single realisation of the Newman–Ziff algorithm we get an estimate of $Q(p)$ for *all* values of p , from 0 to 1.

In our case p_c can be estimated by the value of p at which $Q(p)$ is maximised, since the probability $Q(p)$ tends to zero both for p both above and below p_c , as the system size grows.

For the method to achieve its impressive running time, it is necessary to keep track of clusters efficiently. This can be achieved by a tree based union/find algorithm. For each added edge, we *find* the clusters to which the endpoints belong. If the clusters are different, the *union* of the clusters is calculated. Both steps are rapidly done by representing the set of clusters as a directed forest. By a small modification of the union/find algorithm, detection of cluster wrapping is also easy.

We can speed up the execution by delaying the convolution (equation (2)) and maximisation step, by averaging over a batch of, say m , estimates of $q(n)$ and use the average to estimate $Q(p)$ and p_c . One minor drawback by doing so is that we get fewer samples for estimation the statistical error. Also, the standard error¹ does not decrease as $1/\sqrt{m}$ — but this is only true for small m , and a $1/\sqrt{m}$ factor dominates from $m \approx 10$ and onwards. For the largest system sizes considered here, the standard error for large m is approximately

¹the standard error is an estimate of the standard deviation of the error of the estimate — if the estimator is a mean of n values, the standard error is $s.e. = s/\sqrt{n}$ where s is the sample standard deviation.

$2/\sqrt{m}$ times that for $m = 1$. We thus lose only a factor 2 which is cheap considering that the convolution and maximisation step can be of an order of 100 times more time consuming than the generation step.

We have also run short simulations with the hull gradient method (see for example [7]), using different representations (of the covering graphs) of the lattices, to verify the implementations. (A reason for not using the hull gradient for longer runs was the memory requirement; the simulations were run on standard desktop computers, simultaneously used in daily work by the author's colleagues.)

3. NUMERICAL RESULTS

The finite size error decreases very fast. For our benchmark case, the hexagonal lattice, the finite size bias was of order 10^{-8} for systems of size 50 000.

This prompted us to concentrate the computations on only one large system per lattice. We used square shaped subgraphs, with between 60 000 and 75 000 edges, for which we believe the finite size errors to be of order 10^{-8} , an order of magnitude smaller than the statistical errors. The results are summarized in Table 1. The standard error given is s_m/\sqrt{m} where s_m is the sample standard deviation when m iterations are used for each maximisation step. If we do n realisations, s_m is given by

$$s_m^2 = \frac{1}{N-1} \sum_{i=1}^n (\hat{p}_c^{(i)} - \hat{p}_c)^2,$$

where $\hat{p}_c^{(i)}$ is the estimate from realisation i and \hat{p}_c is the grand estimate, the mean of the $\hat{p}_c^{(i)}$. Approximate $(1 - \alpha)\%$ confidence intervals are given by

$$\hat{p}_c \pm z_{\alpha/2} \text{ s.e.},$$

where $z_{\alpha/2}$ is the $\alpha/2$ quantile of the Gaussian distribution.² For all lattices we used batches of 10^5 realisations for each maximisation step.

In [2], it was observed that the standard deviation scales as

$$\sigma \sim M^{-3/8},$$

where M is the system size (the number of edges). In our simulations we generally observe slightly slower convergence. Fitting $\sigma = CM^{-a}$ we found some variations in the estimated values of a between lattices; we observed values in the range 0.25 to 0.40. The values decrease as the number of iterations m used per maximisation step increases, but appear to settle down for $m \approx 20$. The between-lattice variation also decreases with m . As the purpose here is to get precise estimates for a number of lattices, we have not studied the convergence rate thoroughly for all combinations of lattices and parameters. In Table 1 we report estimates of a for $m = 100$. For the hexagonal lattice, Figure 2 shows a log-log-log plot of the sample standard deviation as a function of system size and number of iterations per maximisation step. The numbers in parenthesis give the estimated values of the exponents a for fixed values of m .

²Strictly speaking t -distribution quantiles should be used, but for the values of n used here they agree with the Gaussian quantiles.

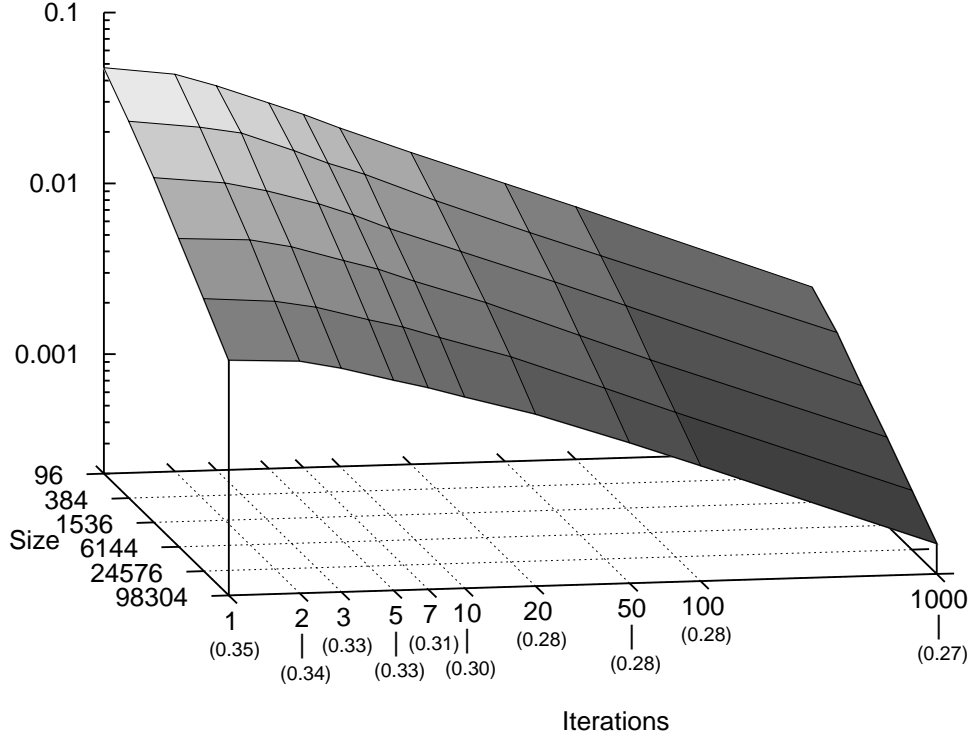


FIGURE 2. Sample standard deviation as function of system size and number of iterations per maximisation step.

TABLE 1. Simulation results. The standard error is denoted by s.e., the number of realizations by n , the system size by M , and the estimated value of the exponent a is denoted by \hat{a} .

Lattice	\hat{p}_c	s.e./ 10^{-7}	n	M	\hat{a}
$(3, 12^2)$	0.740 421 95	8.0	2485	67 500	0.276
$(4, 6, 12)$	0.693 733 83	7.2	2930	73 728	0.277
$(4, 8^2)$	0.676 802 32	6.3	2983	60 000	0.284
$(3, 4, 6, 4)$	0.524 832 58	5.3	7568	64 800	0.286
$(3^4, 6)$	0.434 306 21	5.0	7397	64 000	0.274
$(3^3, 4^2)$	0.419 641 91	4.3	9822	64 000	0.274
$(3^2, 4, 3, 4)$	0.414 137 43	4.6	7504	64 000	0.269

For the hexagonal lattice we did long simulations for 6 different system sizes to study the precision. We used batches of 10^4 realisations. The results are summarized in Table 2. The exact value of the bond percolation threshold is $p_c = 1 - 2 \sin(\pi/18) \approx 0.652\,703\,6446$.

TABLE 2. Simulation results for the hexagonal lattice. Here M denotes the number of edges, n the total number of realizations used for the estimate \hat{p}_c , with standard error s.e. Further, s_1 is the sample standard deviation when one repetition is used for each maximisation step, and s_∞ is an estimate of the limiting sample standard deviation per repetition when m repetitions are used for each maximisation step.

M	$n/10^4$	\hat{p}_c	s.e.	s_1	s_∞
96	754 700	0.652 685 19	6.68×10^{-7}	0.048	0.058
384	634 300	0.652 707 81	5.38×10^{-7}	0.032	0.043
1536	460 520	0.652 704 77	4.49×10^{-7}	0.021	0.030
6144	444 786	0.652 703 77	3.12×10^{-7}	0.013	0.021
24 576	41 727	0.652 703 87	6.58×10^{-7}	0.0079	0.014
98 304	5326	0.652 703 67	1.32×10^{-6}	0.0048	0.0097

The small finite size bias observed in [2] is confirmed by our simulations. The estimates \hat{p}_c are conjectured to converge like

$$|\hat{p}_c - p_c| \sim M^{-11/8}.$$

Fitting

$$\hat{p}_c = p_c + bM^{-11/8}$$

to data, excluding the $M = 96$ data point, gives $b = 0.0017$ and a finite size error for $M = 50\,000$ of 3.4×10^{-8} .

Excluding further data points for small values of M gives slight variations, but the finite size error is always below 4×10^{-8} . This supports our belief that the finite size error for our main estimates are considerable less than the statistical error.

It is also worthwhile to note that, except for very small sizes, the finite size bias is positive, in contrast to the site percolation case studied in [2]. (The same is observed with the hull gradient method; for the bond cases studied here, the finite size bias is positive, while the site cases on the same lattices studied in [7] have negative finite size biases.)

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